

Data File : H:\VOL1\GCMSDATA\J\120720\BJ001035.D

Vial: 2

Acq On : 20 Jul 2012 11:49

Operator: HLM

Sample : CWA-6

Inst : BNA J

Misc : BNA J HLM

Multiplr: 1.00

MS Integration Params: rteint.p

Quant Time: Jul 20 13:58 2012

Quant Results File: BJ072012.RES

Quant Method : H:\VOL1\GCMSDATA\J\METHODS\BJ072012.M (RTE Integrator)

Title : CWA degradation products by GCMS

Last Update : Fri Jul 20 13:59:18 2012

Response via : Initial Calibration

DataAcq Meth : CWAJ

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	4.67	152	44382	2.00	ug/mL	0.00
6) Naphthalene-d8	5.96	136	200975	2.00	ug/mL	0.01

System Monitoring Compounds

10) Tripropylphosphate	7.00	99	1532524	19.53	ug/mL	0.00
Spiked Amount	0.500	Range	70 - 130	Recovery	= 3906.00%#	
12) 2-Bromothioanisole	7.26	204	1706793	124.38	ug/mL	0.01
Spiked Amount	5.000	Range	70 - 130	Recovery	= 2487.60%#	

Target Compounds

					Ovalue
2) Dimethyl Disulfide	2.55	94	907079	60.20	ug/mL# 81
3) DMMP	3.60	79	1210968	71.95	ug/mL 99
4) DIMP	4.97	97	578888	15.26	ug/mL 97
5) 1,4-Oxathiane	3.73	46	3178123	214.44	ug/mL 97
7) 1,4-Dithiane	5.11	46	510218	35.64	ug/mL# 61
8) Thiodiglycol	5.94	61	5356319	286.26	ug/mL 95
9) Benzothiazole	6.26	135	4664905	84.50	ug/mL 97
11) p-Chlorophenylmethyldisulfide	6.51	158	2770560	79.93	ug/mL 87
13) p-Chlorophenylmethyldisulfox	7.93	159	2070361	60.37	ug/mL 83
14) p-Chlorophenylmethyldisulfon	8.14	111	3490701	119.36	ug/mL 90

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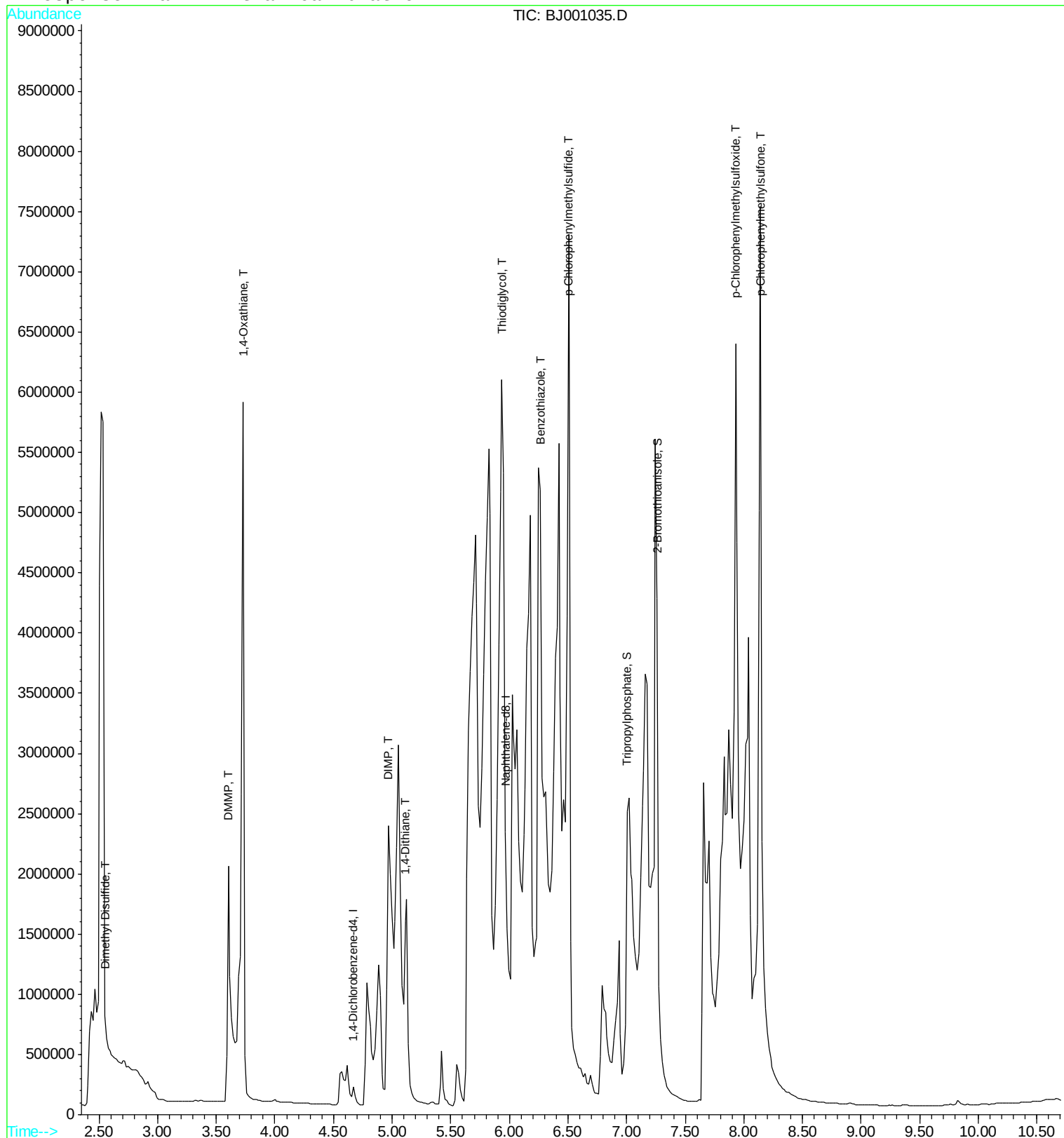
Quant Results File: BJ072012.RES

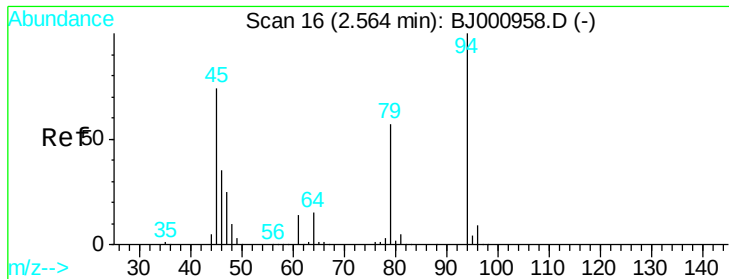
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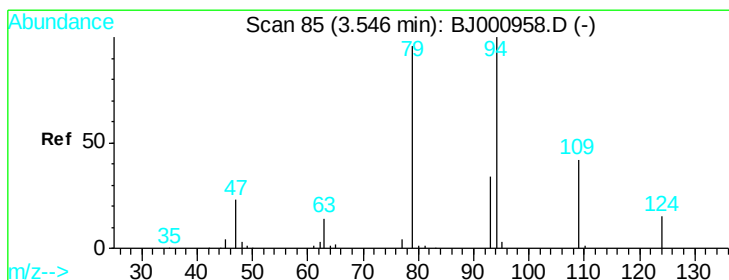
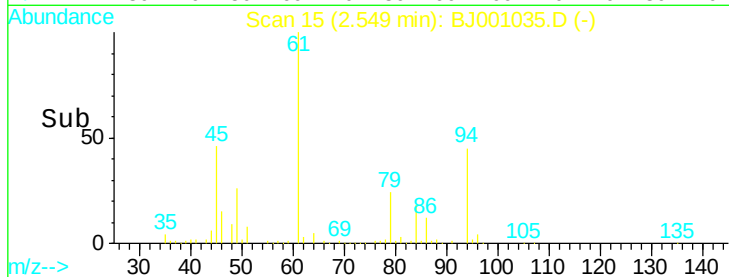
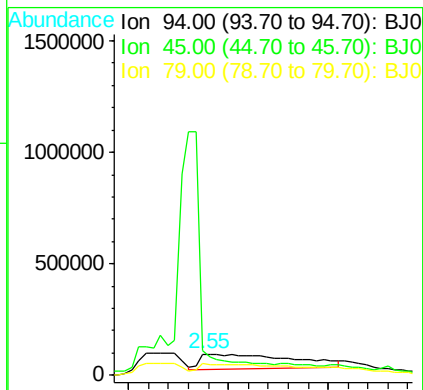
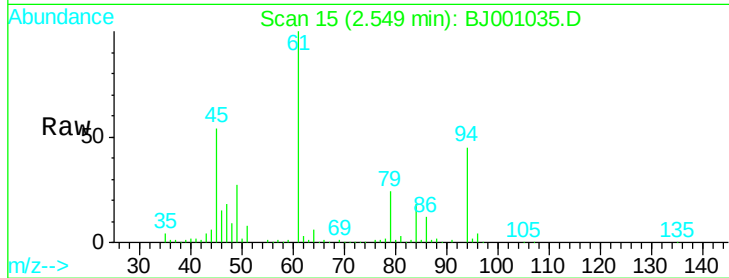




#2

Dimethyl Disulfide
Concen: 60.20 ug/mL
RT: 2.55 min Scan# 15
Delta R.T. -0.03 min
Lab File: BJ001035.D
Acq: 20 Jul 2012 11:49

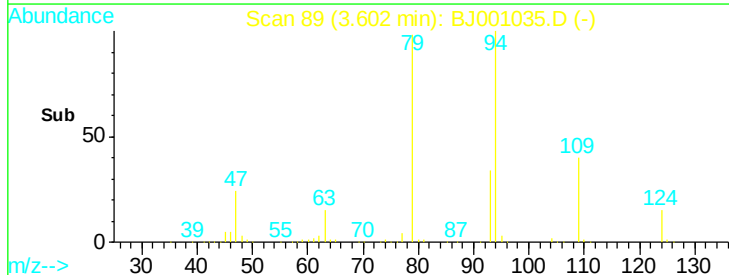
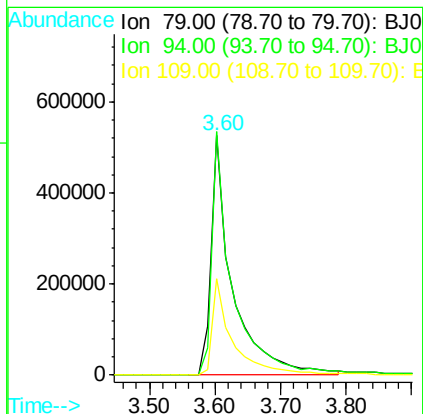
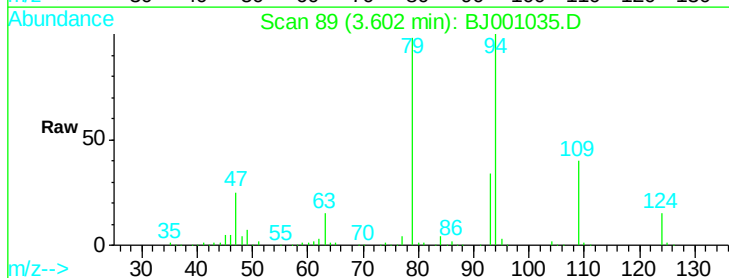
Tgt Ion: 94 Resp: 907079
Ion Ratio Lower Upper
94 100
45 118.8 75.2 115.2#
79 53.6 43.1 83.1

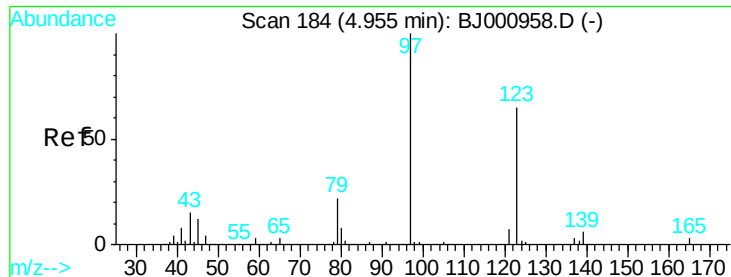


#3

DMMP
Concen: 71.95 ug/mL
RT: 3.60 min Scan# 89
Delta R.T. 0.06 min
Lab File: BJ001035.D
Acq: 20 Jul 2012 11:49

Tgt Ion: 79 Resp: 1210968
Ion Ratio Lower Upper
79 100
94 101.6 83.0 123.0
109 40.4 20.0 60.0





#4

DIMP

Concen: 15.26 ug/mL

RT: 4.97 min Scan# 185

Delta R.T. 0.03 min

Lab File: BJ001035.D

Acq: 20 Jul 2012 11:49

Tgt Ion: 97 Resp: 578888

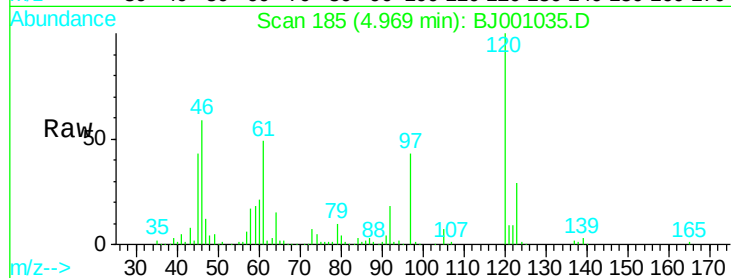
Ion Ratio Lower Upper

97 100

123 66.5 43.8 83.8

43 18.3 0.0 38.6

41 12.3 0.0 29.1



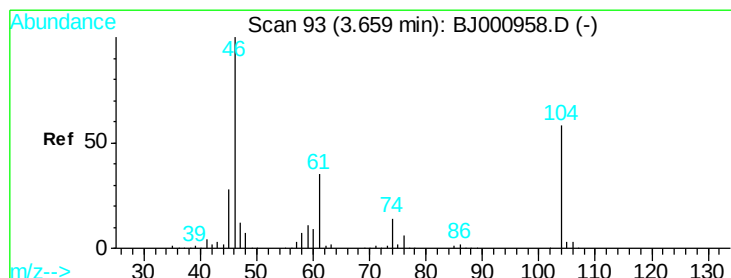
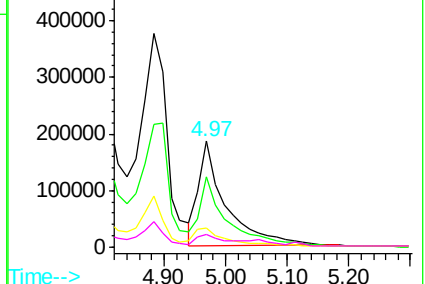
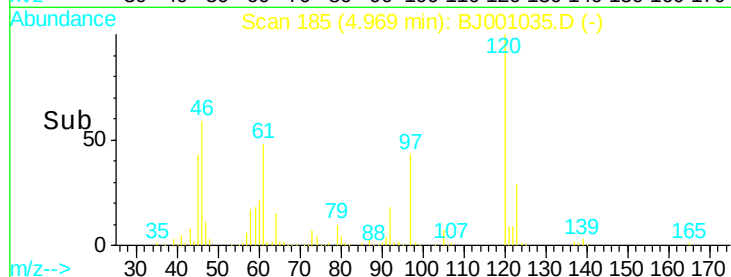
Abundance

Ion 97.00 (96.70 to 97.70): BJ0

Ion 123.00 (122.70 to 123.70): BJ0

Ion 43.00 (42.70 to 43.70): BJ0

Ion 41.00 (40.70 to 41.70): BJ0



#5

1,4-Oxathiane

Concen: 214.44 ug/mL

RT: 3.73 min Scan# 98

Delta R.T. 0.08 min

Lab File: BJ001035.D

Acq: 20 Jul 2012 11:49

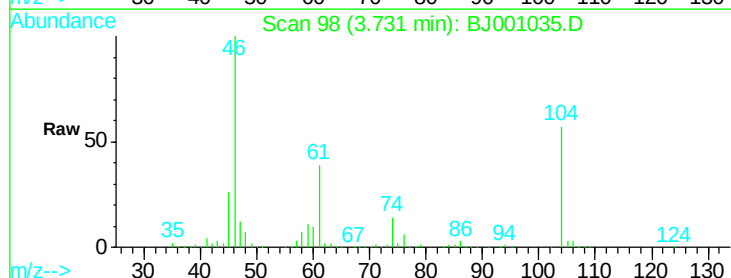
Tgt Ion: 46 Resp: 3178123

Ion Ratio Lower Upper

46 100

61 38.5 19.4 59.4

104 57.2 34.1 74.1

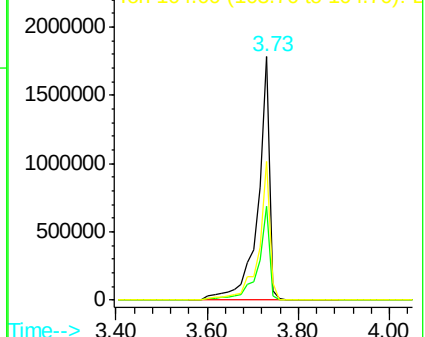
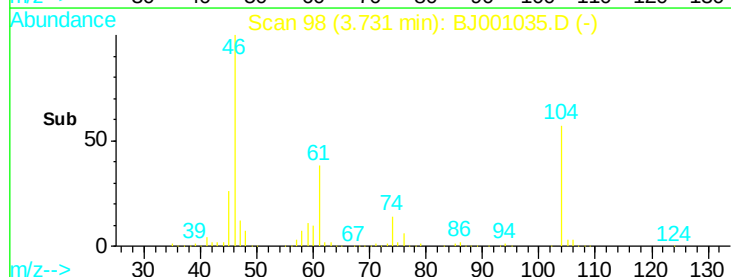


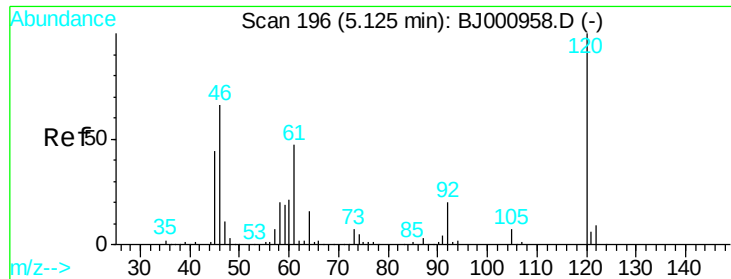
Abundance

Ion 46.00 (45.70 to 46.70): BJ0

Ion 61.00 (60.70 to 61.70): BJ0

Ion 104.00 (103.70 to 104.70): BJ0





#7

1,4-Dithiane

Concen: 35.64 ug/mL

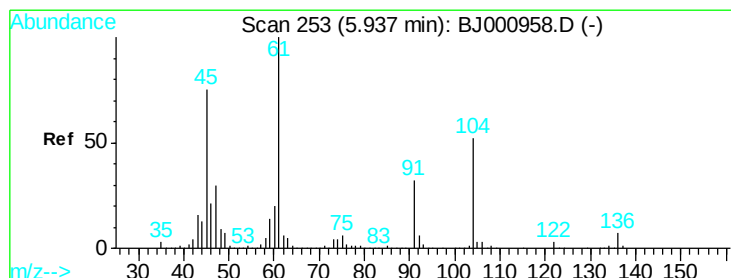
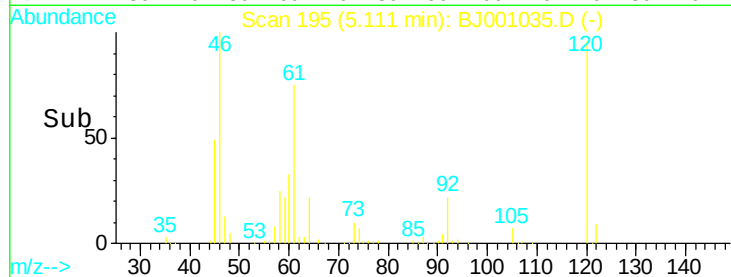
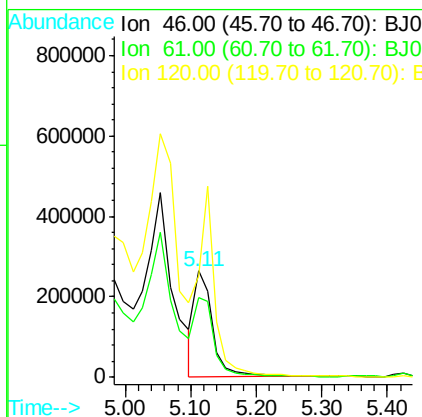
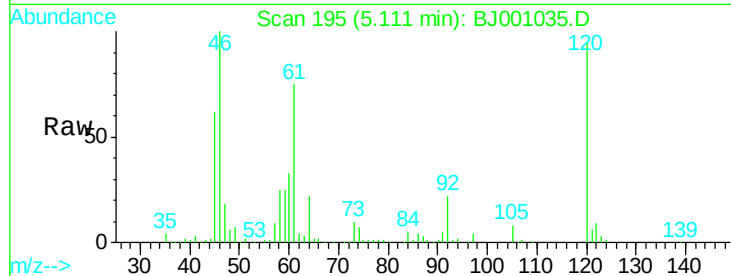
RT: 5.11 min Scan# 195

Delta R.T. -0.00 min

Lab File: BJ001035.D

Acq: 20 Jul 2012 11:49

Tgt Ion:	46	Resp:	510218
Ion	Ratio	Lower	Upper
46	100		
61	74.6	63.7	103.7
120	95.3	148.0	188.0#



#8

Thiodiglycol

Concen: 286.26 ug/mL

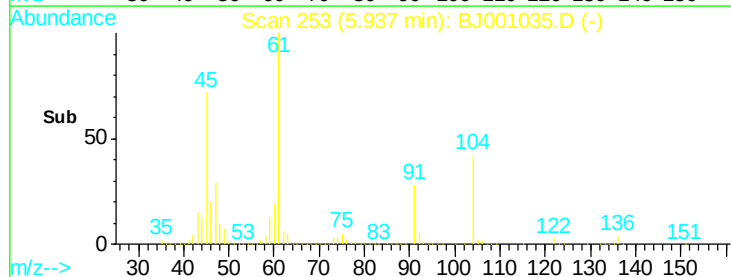
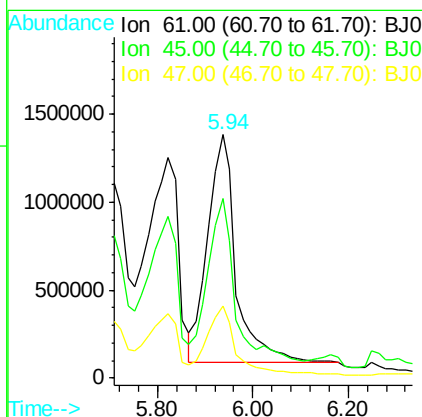
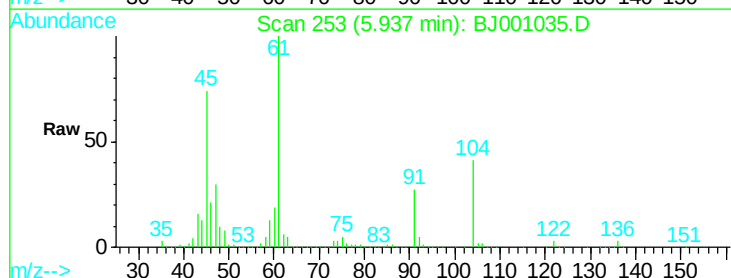
RT: 5.94 min Scan# 253

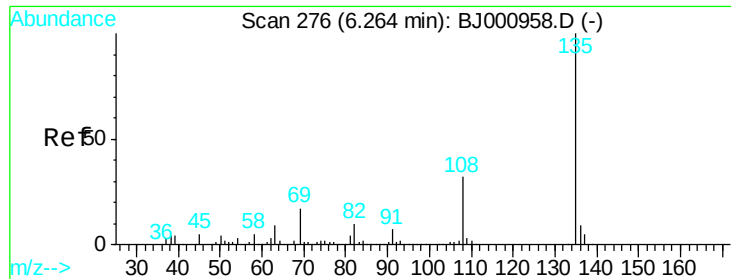
Delta R.T. 0.01 min

Lab File: BJ001035.D

Acq: 20 Jul 2012 11:49

Tgt Ion:	61	Resp:	5356319
Ion	Ratio	Lower	Upper
61	100		
45	73.7	49.0	89.0
47	29.5	7.6	47.6





#9

Benzothiazole

Concen: 84.50 ug/mL

RT: 6.26 min Scan# 276

Delta R.T. 0.01 min

Lab File: BJ001035.D

Acq: 20 Jul 2012 11:49

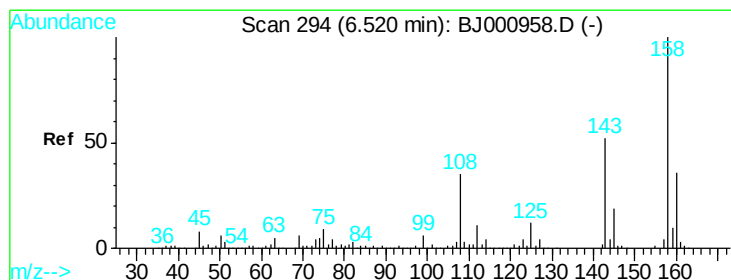
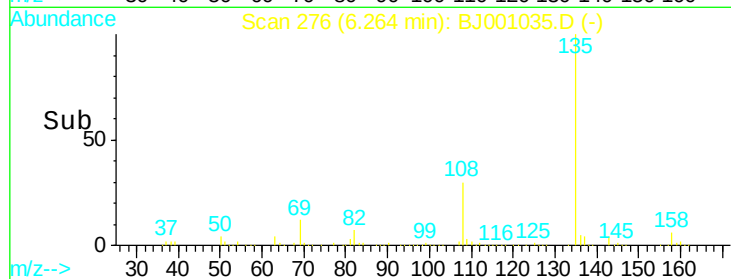
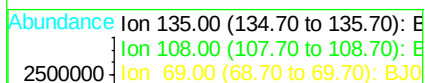
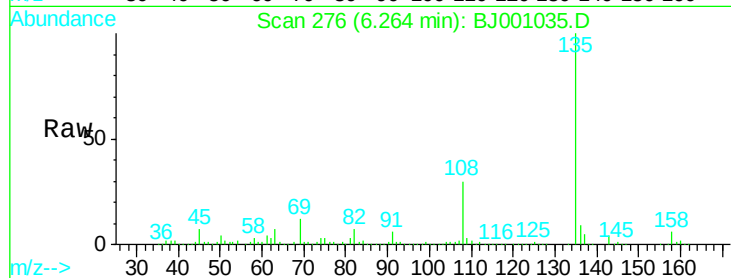
Tgt Ion:135 Resp: 4664905

Ion Ratio Lower Upper

135 100

108 30.5 9.9 49.9

69 12.0 0.0 35.1



#11

p-Chlorophenylmethylsulfide

Concen: 79.93 ug/mL

RT: 6.51 min Scan# 293

Delta R.T. 0.01 min

Lab File: BJ001035.D

Acq: 20 Jul 2012 11:49

Tgt Ion:158 Resp: 2770560

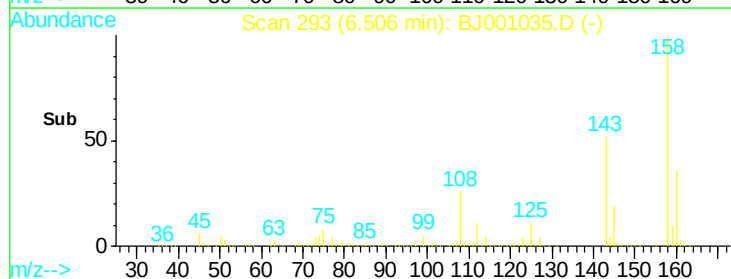
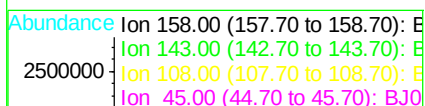
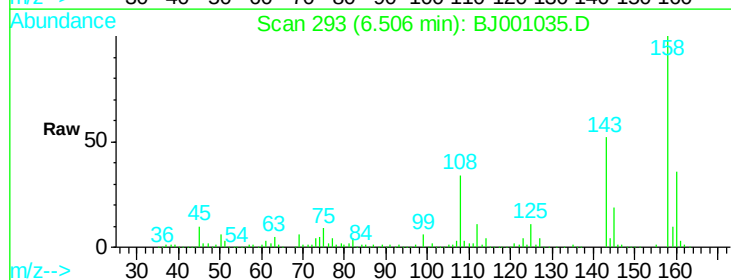
Ion Ratio Lower Upper

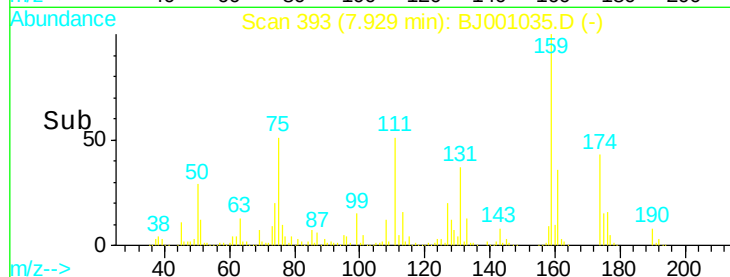
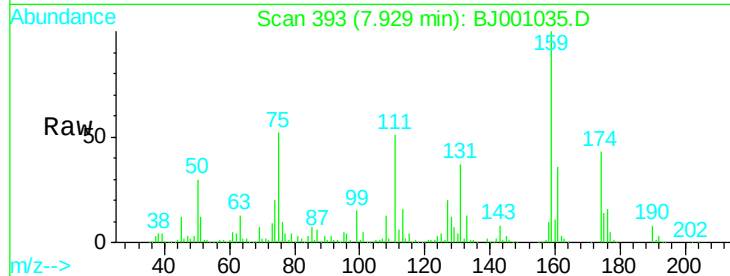
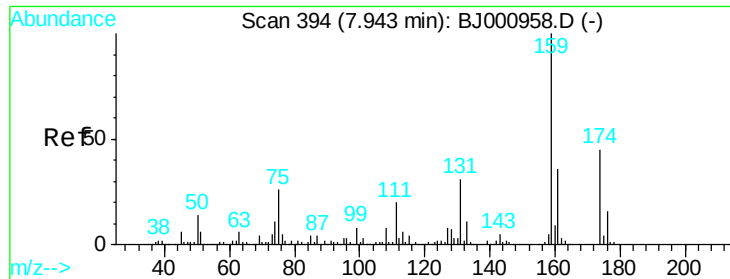
158 100

143 51.6 36.2 76.2

108 34.3 25.5 65.5

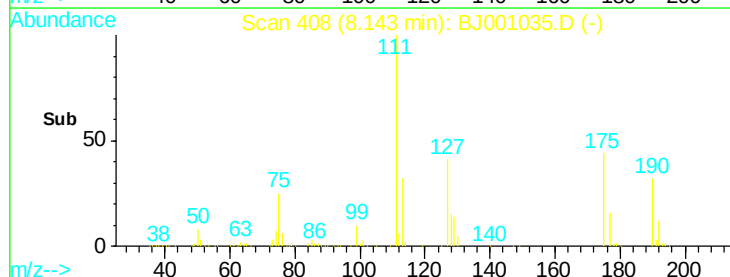
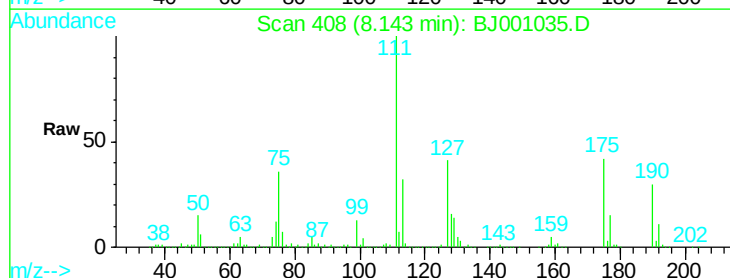
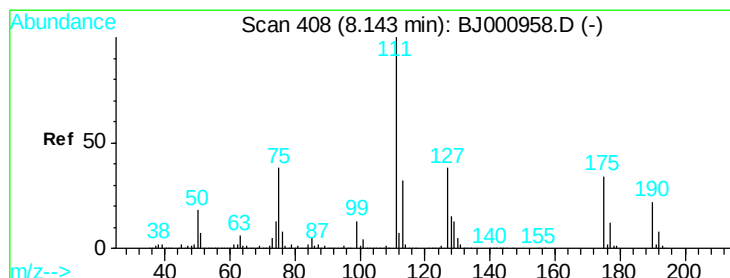
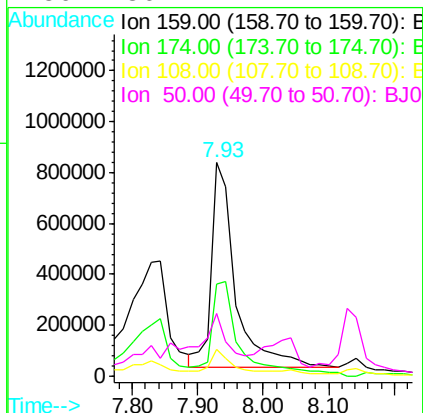
45 9.9 0.7 40.7





#13
p-Chlorophenylmethylsulfoxide
Concen: 60.37 ug/mL
RT: 7.93 min Scan# 393
Delta R.T. -0.00 min
Lab File: BJ001035.D
Acq: 20 Jul 2012 11:49

Tgt Ion:159 Resp: 2070361
Ion Ratio Lower Upper
159 100
174 56.0 27.6 67.6
108 7.0 0.0 31.8
50 36.2 2.7 42.7



#14
p-Chlorophenylmethylsulfone
Concen: 119.36 ug/mL
RT: 8.14 min Scan# 408
Delta R.T. 0.01 min
Lab File: BJ001035.D
Acq: 20 Jul 2012 11:49

Tgt Ion:111 Resp: 3490701
Ion Ratio Lower Upper
111 100
75 35.7 22.6 62.6
127 40.5 17.2 57.2
190 29.5 2.0 42.0

